chain nodes :
    13 17 19 20 21 22 23 26 27 28 29 32 33 35 36 44
ring nodes :
    1 2 3 4 5 6 7 8 9 10 11 12 37 38 39 40 41 42
chain bonds :
    4-7 19-20 20-21 21-22 22-23 26-27 26-28 28-29 32-33 32-35 35-36
ring bonds :
    1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 37-38 37-42 38-39 39-40
    40-41 41-42
exact/norm bonds :
    1-2 1-6 2-3 3-4 4-5 4-7 5-6 19-20 20-21 21-22 22-23 26-27 26-28 28-29 32-33
    32-35 35-36 37-38 37-42
normalized bonds :
    7-8 7-12 8-9 9-10 10-11 11-12 38-39 39-40 40-41 41-42
isolated ring systems :
    containing 1 : 7 : 37 :

G1:CH3,Et

G2:C,N

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 13:CLASS 14:Atom 17:CLASS 18:Atom 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
    26:CLASS 27:CLASS 28:CLASS 29:CLASS 31:Atom 32:CLASS 33:CLASS 34:Atom 35:CLASS
    36:CLASS 37:Atom 38:Atom 39:Atom 40:Atom 41:Atom 42:Atom 44:CLASS 45:Atom 46:Atom